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=> s (nuclear(w)magnetic(w)resonan?)
L1 173424 (NUCLEAR(W) MAGNETIC(W) RESONAN?)

=> s l1 and automat? (4a) assign?
L2 87 L1 AND AUTOMAT? (4A) ASSIGN?

=> dup rem l2
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L3 76 DUP REM L2 (11 DUPLICATES REMOVED)

=> d 1-76 ti

L3 ANSWER 1 OF 76 BIOSIS COPYRIGHT 2002 BIOLOGICAL ABSTRACTS INC.
TI Semi-**automated** backbone resonance **assignments** of the extracellular ligand-binding domain of an ionotropic glutamate receptor.

L3 ANSWER 2 OF 76 MEDLINE DUPLICATE 1
TI Towards structural genomics of RNA: rapid NMR resonance assignment and simultaneous RNA tertiary structure determination using residual dipolar couplings.

L3 ANSWER 3 OF 76 BIOSIS COPYRIGHT 2002 BIOLOGICAL ABSTRACTS INC.
TI Solution structure and dynamics of melanoma inhibitory activity protein.

L3 ANSWER 4 OF 76 MEDLINE
TI Protein NMR structure determination with **automated** NOE **assignment** using the new software CANDID and the torsion angle dynamics algorithm DYANA.

L3 ANSWER 5 OF 76 MEDLINE
TI Self-consistent Karplus parametrization of 3J couplings depending on the polypeptide side-chain torsion chi1.

L3 ANSWER 6 OF 76 MEDLINE
TI Efficient identification of amino acid types for fast protein backbone assignments.

L3 ANSWER 7 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Automatic determination of protein backbone resonance assignments from triple resonance **nuclear magnetic resonance** data

L3 ANSWER 8 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI MUSIC, Selective Pulses, and Tuned Delays: Amino Acid Type-Selective

1H-15N Correlations, II

L3 ANSWER 9 OF 76 MEDLINE
TI Variability in **automated assignment** of NOESY spectra and three-dimensional structure determination: a test case on three small disulfide-bonded proteins.

L3 ANSWER 10 OF 76 MEDLINE
TI Determination of a high precision structure of a novel protein, Linum usitatissimum trypsin inhibitor (LUTI), using computer-aided assignment of NOESY cross-peaks.

L3 ANSWER 11 OF 76 MEDLINE DUPLICATE 2
TI Ansig for Windows: an interactive computer program for semiautomatic assignment of protein NMR spectra.

L3 ANSWER 12 OF 76 MEDLINE
TI Rapid fold and structure determination of the archaeal translation elongation factor 1beta from Methanobacterium thermoautotrophicum.

L3 ANSWER 13 OF 76 MEDLINE
TI RFAC, a program for automated NMR R-factor estimation.

L3 ANSWER 14 OF 76 MEDLINE
TI A tracked approach for **automated** NMR **assignments** in proteins (TATAPRO).

L3 ANSWER 15 OF 76 MEDLINE
TI **Automated** analysis of NMR **assignments** and structures for proteins.

L3 ANSWER 16 OF 76 MEDLINE
TI Solution structure of the VEGF-binding domain of Flt-1: comparison of its free and bound states.

L3 ANSWER 17 OF 76 MEDLINE DUPLICATE 3
TI Exploring protein interiors: the role of a buried histidine in the KH module fold.

L3 ANSWER 18 OF 76 MEDLINE DUPLICATE 4
TI A high quality **nuclear magnetic resonance** solution structure of peptide deformylase from Escherichia coli: application of an **automated assignment** strategy using GARANT.

L3 ANSWER 19 OF 76 MEDLINE DUPLICATE 5
TI New features and enhancements in the X-PLOR computer program.

L3 ANSWER 20 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI RESCUE: an artificial neural network tool for the NMR spectral assignment of proteins

L3 ANSWER 21 OF 76 MEDLINE
TI Structural characterization of an analog of the major rate-determining disulfide folding intermediate of bovine pancreatic ribonuclease A.

L3 ANSWER 22 OF 76 MEDLINE
TI Using neural network predicted secondary structure information in **automatic** protein NMR **assignment**.

L3 ANSWER 23 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI **Automated** Resonance **Assignment** of Proteins Using

Heteronuclear 3D NMR. 2. Side Chain and Sequence-Specific Assignment

L3 ANSWER 24 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI GARANT - a general algorithm for resonance assignment of multidimensional **nuclear magnetic resonance** spectra

L3 ANSWER 25 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Phase labeling of C-H and C-C spin-system topologies: application in constant-time PFG-CBCA(CO)NH experiments for discriminating amino acid spin-system types

L3 ANSWER 26 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Selective identification of threonine, valine, and isoleucine sequential connectivities with a TVI-CBCACONH experiment

L3 ANSWER 27 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI **Automated** sequence-specific NMR **assignment** of homologous proteins using the program GARANT

L3 ANSWER 28 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Use of selective C.alpha. pulses for improvement of HN(CA)CO-D and HN(COCA)NH-D experiments

L3 ANSWER 29 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Phase labeling of C-H and C-C spin-system topologies: application in PFG-HACANH and PFG-HACA(CO)NH triple-resonance experiments for determining backbone resonance assignments in proteins

L3 ANSWER 30 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI A general and adaptable method for the **automated assignment** of protein multidimensional **nuclear magnetic resonance** spectra (NMR)

L3 ANSWER 31 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Automated analysis of **nuclear magnetic resonance** assignments for proteins

L3 ANSWER 32 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI WinDat: An NMR Database Compilation Tool, User Interface, and Spectrum Libraries for Personal Computers

L3 ANSWER 33 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Application of structure refinement using 3D NOE-NOE spectroscopy to lac repressor headpiece (1-56)

L3 ANSWER 34 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI AURELIA, a program for computer-aided analysis of multidimensional NMR spectra

L3 ANSWER 35 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Computer-assisted assignment of peptides with non-standard amino acids

L3 ANSWER 36 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Computer assignment of the backbone resonances of labeled proteins using two-dimensional correlation experiments

L3 ANSWER 37 OF 76 MEDLINE DUPLICATE 6
TI Protein three-dimensional structure determination and sequence-specific assignment of 13C and 15N-separated NOE data. A novel real-space ab initio approach.

L3 ANSWER 38 OF 76 MEDLINE DUPLICATE 7

TI **Automated assignment** of multidimensional **nuclear magnetic resonance** spectra.

L3 ANSWER 39 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Computational strategies pertinent to NMR solution structure determination

L3 ANSWER 40 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Use of fuzzy mathematics for complete **automated assignment** of peptide 1H 2D NMR spectra

L3 ANSWER 41 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI A novel contour plot algorithm for the processing of 2D and 3D NMR spectra

L3 ANSWER 42 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Application of neural networks to **automated assignment** of NMR spectra of proteins

L3 ANSWER 43 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Automation of protein 2D proton NMR assignment by means of fuzzy mathematics and graph theory

L3 ANSWER 44 OF 76 MEDLINE
TI A constraint reasoning system for **automating** sequence-specific resonance **assignments** from multidimensional protein NMR spectra.

L3 ANSWER 45 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Computer-assisted assignment of multidimensional NMR spectra of proteins: Application to 3D NOESY-HMQC and TOCSY-HMQC spectra

L3 ANSWER 46 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI A 4D HCCH-TOCSY experiment for assigning the side chain proton and carbon-13 resonances of proteins

L3 ANSWER 47 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI 4D NMR triple-resonance experiments for assignment of protein backbone nuclei using shared constant-time evolution periods

L3 ANSWER 48 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI RUBIDIUM, a program for computer-aided assignment of two-dimensional NMR spectra of polypeptides

L3 ANSWER 49 OF 76 MEDLINE DUPLICATE 8
TI Comparison of solution structures of mutant bovine pancreatic trypsin inhibitor proteins using two-dimensional **nuclear magnetic resonance**.

L3 ANSWER 50 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Two- and three-dimensional proton NMR studies of apo-neocarzinostatin

L3 ANSWER 51 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Assignment of protein NMR spectra in the light of homonuclear 3D spectroscopy: an automatable procedure based on 3D TOCSY-TOCSY and 3D TOCSY-NOESY

L3 ANSWER 52 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI STELLA and CLAIRE: a seraglio of programs for human-aided assignment of 2D proton NMR spectra of proteins

L3 ANSWER 53 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Assignment of the NMR spectra of homologous proteins

L3 ANSWER 54 OF 76 CAPLUS COPYRIGHT 2002 ACS

TI New interactive and **automatic** algorithms for the **assignment** of NMR spectra

L3 ANSWER 55 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Automated analysis of NMR spectra

L3 ANSWER 56 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Pepto: an expert system for **automatic** peak **assignment** of two-dimensional **nuclear magnetic resonance** spectra of proteins

L3 ANSWER 57 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI A versatile approach toward the partially automatic recognition of cross peaks in 2D proton NMR spectra

L3 ANSWER 58 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Three-dimensional TOCSY-TOCSY processing using linear prediction, as a potential technique for **automated assignment**

L3 ANSWER 59 OF 76 BIOSIS COPYRIGHT 2002 BIOLOGICAL ABSTRACTS INC.DUPLICATE 9
TI **AUTOMATED** STEREOSPECIFIC PROTON NMR **ASSIGNMENTS** AND THEIR IMPACT ON THE PRECISION OF PROTEIN STRUCTURE DETERMINATIONS IN SOLUTION.

L3 ANSWER 60 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Heteronuclear three-dimensional NMR spectroscopy. Natural abundance carbon-13 chemical shift editing of 1H-1H COSY spectra

L3 ANSWER 61 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI A computer search system for similar organic compounds in carbon-13 **nuclear magnetic resonance** data files

L3 ANSWER 62 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI A program for semi-**automatic** sequential resonance **assignments** in protein proton **nuclear magnetic resonance** spectra

L3 ANSWER 63 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Carbon-13 NMR assignments of the bases in oligodeoxynucleotides: an automated procedure using Bayesian statistics

L3 ANSWER 64 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Use of the carbon-13 NMR chemical shift/charge density linear relationship for recognition and ranking of chemical structures

L3 ANSWER 65 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI ISOLOG: a diagnosis system for origin recognition of natural products through isotope analysis

L3 ANSWER 66 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Toward **automated assignment** of **nuclear magnetic resonance** spectra: pattern recognition in two-dimensional correlation spectra

L3 ANSWER 67 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI CSEARCH: a computer program for identification of organic compounds and fully **automated assignment** of carbon-13 **nuclear magnetic resonance** spectra

L3 ANSWER 68 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI **Automatic assignment** of carbon-13 NMR signals based on

the Karplus-Pople equation

L3 ANSWER 69 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI **Automatic** peak **assignments** for in vivo phosphorus-31 NMR spectra

L3 ANSWER 70 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Empirical additive parameter and **automatic assignment** of carbon-13 NMR signals of some aryl and heteroaryl groups. A new criterion for a linear relationship between carbon-13 chemical shifts and charge densities

L3 ANSWER 71 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI **Automatic assignment** of carbon-13 NMR spectra based on the chemical shift/charge density relationship

L3 ANSWER 72 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Computerized analytical system (ASSIGNER) for structure determination of organic compounds

L3 ANSWER 73 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Automatic structural elucidation by carbon-13 NMR: DARC-EPIOS method. Search for a discriminant chemical structure-displacement relationship

L3 ANSWER 74 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Automatic analysis of the NMR spectra of AA'BB' type compounds with the **automatic assignment** of spectral lines

L3 ANSWER 75 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Shift reagent spectra. The automatic determination of relative bound shifts and the **automatic assignement** of signals in the parent spectrum. Effects of concentration, temperature, and solvent on relative bound shifts

L3 ANSWER 76 OF 76 CAPLUS COPYRIGHT 2002 ACS
TI Computer program for automatic interpretation of NMR spectra on the basis of dipolar lanthanide shifts

=> d 44 bib ab

L3 ANSWER 44 OF 76 MEDLINE
AN 96038996 MEDLINE
DN 96038996 PubMed ID: 7584369
TI A constraint reasoning system for **automating** sequence-specific resonance **assignments** from multidimensional protein NMR spectra.
AU Zimmerman D E; Kulikowski C A; Montelione G T
CS Department of Computer Science, Rutgers University, Piscataway, NJ 08854, USA.
NC GM-08339 (NIGMS)
GM-47014 (NIGMS)
SO ISMB, (1993) 1 447-55.
Journal code: 9509125.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 199512
ED Entered STN: 19960124
Last Updated on STN: 19960124
Entered Medline: 19951205
AB AUTOASSIGN is a prototype expert system designed to aid in the

determination of protein structure from **nuclear magnetic resonance** (NMR) measurements. In this paper we focus on one of the key steps of this process, the assignment of the observed NMR signals to specific atomic nuclei in the protein; i.e. the determination of sequence-specific resonance assignments. Recently developed triple-resonance (1H, 15N, and 13C) NMR experiments [Montelione et al., 1992] have provided an important breakthrough in this field, as the resulting data are more amenable to automated analysis than data sets generated using conventional strategies [Wuethrich, 1986]. The "assignment problem" can be stated as a constraint satisfaction problem (CSP) with some added complexities. There is very little internal structure to the problem, making it difficult to apply subgoaling and problem decomposition. Moreover, the data used to generate the constraints are incomplete, non-unique, and noisy, and constraints emerge dynamically as analysis progresses. The traditional inference engine is replaced by a set of very tightly-coupled modules which enforce extensive constraint propagation, with state information distributed over the objects whose relationships are being constrained. AUTOASSIGN provides correct and nearly complete resonance assignments with both simulated and real 3D triple-resonance data for a 72 amino acid protein.

=> d 38 bib ab

L3 ANSWER 38 OF 76 MEDLINE DUPLICATE 7
AN 95131767 MEDLINE
DN 95131767 PubMed ID: 7830588
TI **Automated assignment** of multidimensional **nuclear magnetic resonance** spectra.
AU Oschkinat H; Croft D
CS European Molecular Biology Laboratory, Germany.
SO METHODS IN ENZYMOLOGY, (1994) 239 308-18. Ref: 41
Journal code: 0212271. ISSN: 0076-6879.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 199502
ED Entered STN: 19950307
Last Updated on STN: 19950307
Entered Medline: 19950217

=> d 15 bib ab

L3 ANSWER 15 OF 76 MEDLINE
AN 1999439930 MEDLINE
DN 99439930 PubMed ID: 10508776
TI **Automated** analysis of NMR **assignments** and structures for proteins.
AU Moseley H N; Montelione G T
CS Center for Advanced Biotechnology and Medicine Department of Molecular Biology and Biochemistry, Rutgers University, Piscataway, New Jersey, 08854-5638, USA.. hunter@cabm.rutgers.edu
NC GM-47014 (NIGMS)
SO CURRENT OPINION IN STRUCTURAL BIOLOGY, (1999 Oct) 9 (5) 635-42. Ref: 42
Journal code: 9107784. ISSN: 0959-440X.
CY ENGLAND: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)

(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 199911
ED Entered STN: 20000111
Last Updated on STN: 20000111
Entered Medline: 19991105
AB Recent developments in protein NMR technology have provided spectral data that are highly amenable to analysis by advanced computer software systems. Specific data collection strategies, coupled with these computer programs, allow automated analysis of extensive backbone and sidechain resonance assignments and three-dimensional structures for proteins of 50 to 200 amino acids.

=> d 18 bib ab

L3 ANSWER 18 OF 76 MEDLINE DUPLICATE 4
AN 1999281460 MEDLINE
DN 99281460 PubMed ID: 10353194
TI A high quality **nuclear magnetic resonance** solution structure of peptide deformylase from Escherichia coli: application of an **automated assignment** strategy using GARANT.
AU O'Connell J F; Pryor K D; Grant S K; Leiting B
CS Department of Biochemistry, Merck Research Laboratories, Rahway, NJ 07065, USA.. oconnell@merck.com
SO JOURNAL OF BIOMOLECULAR NMR, (1999 Apr) 13 (4) 311-24.
Journal code: 9110829. ISSN: 0925-2738.
CY Netherlands
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 199906
ED Entered STN: 19990712
Last Updated on STN: 20000303
Entered Medline: 19990624
AB The NMR structure of the peptide deformylase (PDF) (1-150) from Escherichia coli, which is an essential enzyme that removes the formyl group from nascent polypeptides and represents a potential target for drug discovery, was determined using 15N/13C doubly labeled protein. Nearly completely **automated assignment** routines were employed to assign three-dimensional triple resonance, 15N-resolved and 13C-resolved NOESY spectra using the program GARANT. This assignment strategy, demonstrated on a 17 kDa protein, is a significant advance in the **automation** of NMR data **assignment** and structure determination that will accelerate future work. A total of 2302 conformational constraints were collected as input for the distance geometry program DYANA. After restrained energy minimization with the program X-PLOR the 20 best conformers characterize a high quality structure with an average of 0.43 A for the root-mean-square deviation calculated from the backbone atoms N, C alpha and C', and 0.81 A for all heavy atoms of the individual conformers relative to the mean coordinates for residues 1 to 150. The globular fold of PDF contains two alpha-helices comprising residues 25-40, 125-138, six beta-strands 57-60, 70-77, 85-88, 98-101, 105-111, 117-123 and one 3(10) helix comprising residues 49-51. The C-terminal helix contains the HEXXH motif positioning a zinc ligand in a similar fashion to other metalloproteases, with the third ligand being cysteine and the fourth presumably a water. The three-dimensional structure of PDF affords insight into the substrate recognition and specificity for N-formylated over N-acetylated substrates and is compared to other PDF structures.

=> d 24, 27, 30, 31 bib ab

L3 ANSWER 24 OF 76 CAPLUS COPYRIGHT 2002 ACS
AN 1997:10368 CAPLUS
DN 126:138925
TI GARANT - a general algorithm for resonance assignment of multidimensional **nuclear magnetic resonance** spectra
AU Bartels, Christian; Guentert, Peter; Billeter, Martin; Wuethrich, Kurt
CS Institut Molekularbiologie Biophysik, Eidgenoessische Technische Hochschule-Hoenggerberg, Zurich, CH-8093, Switz.
SO Journal of Computational Chemistry (1997), 18(1), 139-149
CODEN: JCCHDD; ISSN: 0192-8651
PB Wiley
DT Journal
LA English
AB A new program for **automatic** resonance **assignment** of NMR spectra of proteins, GARANT (General Algorithm for Resonance Assignment), is introduce. Three principal elements used in this approach are: (a) representation of resonance assignments as an optimal match of two graphs describing, resp., peaks expected from combined knowledge of the primary structure and the magnetization transfer pathways in the spectra used, and exptl. obsd. peaks; (b) a scoring scheme able to distinguish between correct and incorrect resonance assignments; and (c) combination of an evolutionary algorithm with a local optimization routine. The score that valuates the match of expected peaks to obsd. relies on the agreement of the information available about these peaks, most prominently, but not exclusively, the chem. shifts. Tests show that the combination of an evolutionary algorithm and a local optimization routinely results that are clearly superior to those obtained when using either of the two techniques sep. in the search for the correct assignments. GARANT is laid out for assignment problems involving peaks obsd. in two- and three-dimensional homonuclear and heteronuclear NMR spectra of proteins.

L3 ANSWER 27 OF 76 CAPLUS COPYRIGHT 2002 ACS
AN 1996:408828 CAPLUS
DN 125:137103
TI **Automated** sequence-specific NMR **assignment** of homologous proteins using the program GARANT
AU Bartels, Christian; Billeter, Martin; Guentert, Peter; Wuethrich, Kurt
CS Inst. Mol. Biophysik, Eidgenoessische Technische Hochschule-Hoenggerberg, Zurich, CH-8093, Switz.
SO Journal of Biomolecular NMR (1996), 7(3), 207-213
CODEN: JBNME9; ISSN: 0925-2738
PB ESCOM
DT Journal
LA English
AB The program GRANT (General Algorithm for Resonance **Assignment**) for **automated** sequence-specific NMR **assignment** of proteins is based on the mapping of peaks predicted from the amino acid sequence onto the peaks obsd. in multidimensional spectra (1996). In this paper we demonstrate the potential of GARANT for the assignment of homologous proteins when either the three-dimensional structure or the chem. shifts of the parent protein are known. In these applications, GARANT utilizes supplementary information either in the form of interat. distances derived from the three-dimensional structure, to add nuclear Overhauser effects reflecting the tertiary structure to the list of expected peaks, or in the form of the chem. shifts of the parent protein, to obtain a better est. of the positions of the expected peaks. The procedure is illustrated with three different proteins: (i) a mutant form

of Tendamistat (74 residues), using homonuclear 2D 1H NMR spectra and either the three-dimensional structure or the chem. shifts of the wild-type protein; (ii) the mutant Antp(C39S,W56S) homeodomain (68 residues), using homonuclear 2D 1H NMR spectra and the three-dimensional structure of the Antp(C39S) homeodomain; and (iii) free cyclophilin A (165 residues), using heteronuclear 3D NMR spectra and the three-dimensional structure of a cyclophilin A-cyclosporin A complex. In these three systems nearly complete assignment of the polypeptide backbone resonances and assignment of over 80% of the amino acid side-chain resonances was obtained without manual intervention.

L3 ANSWER 30 OF 76 CAPLUS COPYRIGHT 2002 ACS
AN 1996:408812 CAPLUS
DN 125:77742
TI A general and adaptable method for the **automated assignment** of protein multidimensional **nuclear magnetic resonance** spectra (NMR)
AU Olson, John Bernard, Jr.
CS Univ. of Wisconsin, Madison, WI, USA
SO (1995) 216 pp. Avail.: Univ. Microfilms Int., Order No. DA9608152
From: Diss. Abstr. Int., B 1996, 57(1), 309
DT Dissertation
LA English
AB Unavailable

L3 ANSWER 31 OF 76 CAPLUS COPYRIGHT 2002 ACS
AN 1995:911855 CAPLUS
DN 123:309747
TI Automated analysis of **nuclear magnetic resonance** assignments for proteins
AU Zimmerman, Diane E.; Montelione, Gaetano T.
CS Rutgers Univ., Piscataway, NJ, USA
SO Current Opinion in Structural Biology (1995), 5(5), 664-73
CODEN: COSBEF; ISSN: 0959-440X
PB Current Biology
DT Journal
LA English
AB Recent developments in protein NMR technol. provide spectral data that are highly amenable to anal. by computer software systems. Automated methods of anal. use constraint satisfaction, pseudoenergy minimization, directed search, neural net, simulated annealing, and/or genetic algorithms to establish sequential links and sequence-specific assignments. The most advanced systems provide automated anal. of complete backbone and extensive side-chain resonance assignments for proteins of 50-150 amino acids.

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